Subject index

Ab initio 377
Adiabatic corrections 249
All-trans conjugated polyenes 155
AtH 351
Atomic dipole polarizabilities of Pb, Bi, Po, and At 351

BeAr 209
Benzene 377
Benzene heteroatom analogues 57
BiH_3 351
Biorthogonal representation 339
Bond orders 57
Bonding 57, 201
Bond-breaking processes 123
BSSE 377

Carbon 455
Carbon clusters 227, 367
Cartesian Gaussians 441
CASSCF 209
Catchment regions 433
Ca_3/Ca_4 metallic clusters 165
CCSD(T) method 165
CdAr 209
Charges 319
CI calculations 123
CI limit 31
Counterpoise correction 377
Coupled-cluster approach 69
CPHF 455
Cu_2 201
C_{60} 367
C_{60}–C_{70} 455
C_{70} 367
C_8/C_{10} 227

Derivative integrals 117
Dihalides 239
Dipole moments and polarizabilites of the fifth-row hydrides 351
Direct 455
Dynamic resonance 331
Dynamic σ-π polarization 191
d-*d*-excitation spectra 389

Effective core potential method 239
Effective Hamiltonian 389
Electron correlation energy 239
Electron density 185
Electron interaction integrals 105
Electronic structure 389
Electronic structure calculations 227
Energy derivatives 117
Energy expectation value 264
Equilibrium geometries 227
Excited states 209
Exponentially decaying functions 105

Fullerene 367

Gaussian integrals 177
GIAO 455
Global vs. local energy minima 257
Gradient extremals 15
Gradients 117
Graphical methods of spin algebras 69
Ground states 209

Halogen halides 239
Hermite functions 441
Hiller-Sucher-Feinberg identity 185
Hirshfeld population analysis 319
Hückel theory 313
Hypervirial theorem 185
H+HCl 331
H_2 (hydrogen molecule) 249

IRC 433
Isomeric interplay at finite temperatures 257
$i\,^3\Pi_g$ state 249

K_2 201

Leapfrog transformation 367
Lie algebra 264

LMO 123
„Local" moments 319

Magnetic shielding 455
Many-electron correlation problem 69
MC-SCF 191
MgAr 209
Model potential method 239
Molecular density 319
Molecular electric properties 351
Molecular two-electron integrals 441
Moments 313
MRCI 191
Multiple energy minima 257
Multipole expansion 185
Multi-reference formalism 69

Na_2 201
NMR 455
Nuclear attraction 105

Orbital optimization 339
OsH_2 141

Pentacoordinated molecules 21
Perturbation theory 264
PbH_4 351
PH_4F 21
PoH_2 351
Polarizability 455
Polarized basis sets 351
Polaron- and bipolaron-like defects 155
Polyenes, *all-trans* conjugated 155
Potential energy surface 433
Potential energy surfaces 15, 141
Pseudorotation 21

Reaction paths 15
Recoupling procedures 417
Relativistic contributions to atomic and molecular properties 351
Relativistic effects 141
Resonance energy 377
r_{12} methods 441

Saddle point 433
Saddle points 15
Spin-adaptation 69
Stationarity 264
Stationary points of potential hypersurfaces 257
Symmetry 367
Systematic sequences of wavefunctions 31

Theory/experiment comparisons 257
Total π-electron energy 313
Transition metal complexes 389

Unitary group approach 417

Valence bond theory 339
Valence *p* functions 201
Variational approach 264
Vibrational frequencies 165

Wavefunctions, full CI limit 31
Weyl tableau basis states 417